

Collaborative Research on Large-Scale Dislocation Dynamics Simulations For Computational Design of Semiconductor Thin Film Systems

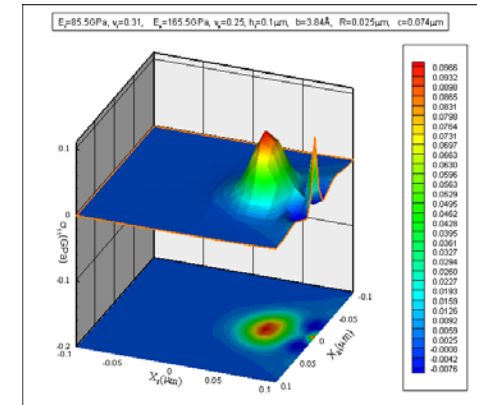
Lizhi Sun, The University of Iowa, DMR 0113172

Epitaxial thin film heterostructures are pervasive in modern applications including microelectronics, magnets, and optics. However, the presence of defects (e.g., dislocations) significantly degrades the mechanical, electrical and optical properties of thin films.

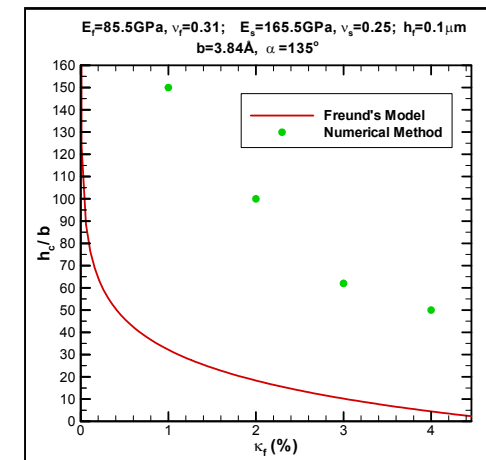
We developed the stress field calculation induced by arbitrary dislocation loops in thin-film heterostructures. With the eigenstrain theory, we also derived an analytical solution to the lattice-misfit strain problem.

We further proposed a 3-D method to dislocation dynamics simulation, in which free surface and interface effects were rigorously addressed. The model was able to estimate the initial dislocation geometry for growth and the critical thickness of thin films.

Two Ph.D. students (E. Tan and H. Liu) are contributing to this work. Research results are implemented to the graduate-level micromechanics course.



Stress field induced by dislocations interacting with interface/surface.



Critical thickness of thin films